

## Map, Measure, and Model

All of the processes alluded to here (water infiltration, corrosion, transport through unsaturated and saturated rock, etc.) were investigated in great detail. As a small example, of the 7 inches of rain that falls annually on Yucca Mountain, scientists learned that only about 5 percent is absorbed by the thirsty mountain. The rainwater then takes thousands of years to percolate through the mountain, but small amounts (less than 0.1 percent) could reach the repository in only decades by flowing along cracks or fault lines.

Los Alamos scientists contributed heavily to much of the research and were instrumental in evaluating how the waste particles move through unsaturated and saturated rock. Los Alamos staff also wrote or co-wrote five sections of the license application, those pertaining to climate and infiltration (Dan Levitt), waste package and drip-shield corrosion (Neil Brown), radionuclide transport in the unsaturated zone (Bruce Robinson), flow and transport in the saturated zone (Ken Rehfeldt), and igneous activity (Frank Perry).

Along with scientists and engineers from the Sandia, Lawrence Berkeley, and Lawrence Livermore national laboratories and other institutions, Los Alamos scientists constructed numerical models of water flow and radionuclide transport through the mountain and conducted many of the basic field investigations and laboratory experiments needed to measure the parameters that go into those models.

But regardless of the skill of the experimenter, the parameters were not and could not be measured with complete certainty.

"It's the uncertainties in the parameters that raised lots of eyebrows," says Dixon. "People asked how we could know if the models are correct, and hence extendable to a million years, if the parameters aren't understood fully."

He responds that because of the uncertainties, every model gets developed for a range of parameter values. And while the exact value of a parameter is uncertain, the range of values (the parameter "space") is known quite well. Plugging a range of values into the process models can demonstrate that the conclusions drawn from the TSPA model don't change, regardless of the uncertainty of its parameters. "Within the ranges that are applicable to the repository, the mountain, and the region, we know the models are reliable," says Dixon.

Even so, once the repository is built, DOE will continue to conduct performance-confirmation tests that ensure the models are sufficiently accurate. The repository won't be sealed off for its first 100 years or so. While no one expects a startling "oops" that requires a rethinking of the repository's design, assessing real repository performance is the prudent thing to do.

Will the repository at Yucca Mountain be built? For Robinson, that's a societal and political decision that doesn't affect his going to work each morning.

"Our job is to make sure that whatever the decision is, it's informed by science," says Robinson. "It's the complete scientific case, not simply the numbers that come out of a computer model, that provides the evidence needed for the decision. Even though natural systems are messy, complex, and uncertain, we've conducted our repository science within the structure of total system performance assessments, which show that the repository will comfortably meet the full set of regulatory requirements. That's why I believe it's safe."

### FEHM: One Code, Many Uses

During the late 1970s, when the Laboratory's Hot Dry Rock geothermal energy project at Fenton Hill was trying to heat water by drilling deep into the earth and tapping its high temperatures (250°C–300°C), George Zyvoloski was trying to figure out just how hot the water would get as it circulated through an underground heat exchanger. Zyvoloski had a pioneering idea: find the answer by using Los Alamos' world-class supercomputers and computational facilities to solve the equations that govern how heat and mass are transported through porous media. The computer code that he began using was called Finite Element Heat and Mass, or FEHM.

"I remember submitting jobs on the Lab's Cray-1 supercomputer," says Zyvoloski, "and competing with others who were queuing up to access the Cray's awesome 133 megaflops of processing power and 8 megabytes of main memory. I was trying to understand the rate at which heat would be extracted from the rocks. The simulations proved to be essential." Zyvoloski and others realized the inherent power of using numerical models to simulate the transport of heat, mass, and chemical constituents in porous media. They further realized that by focusing on the general set of transport equations, rather than on equations geared toward a particular application, major advances could be made in many different research areas.

The Yucca Mountain project made extensive use of FEHM to simulate how radionuclides might migrate through the mountain's porous rock. Broad new capabilities had been added to the initial code, including ways to simulate multiple fluid phases and ways to account for chemical processes that arose from interactions between fluids and minerals. So-called inverse modeling methods, in which the computer model is automatically adjusted until its output matches the available data (instead of simply running the model to see what one gets) became part of the code's repertoire. These methods were especially advantageous to project scientists in that they would help quantify the uncertainty in the model's predictions. Today FEHM helps researchers model and understand many phenomena, including the movement of actinides in the groundwater beneath Los Alamos, the sequestration of carbon dioxide in deep saline aquifers, the extraction of organic compounds from oil shale, and the potential use of methane hydrates to meet our future energy needs. It's a commonly used code that is uncommonly good for solving problems.